# Dynamic Approach to Weak First Order Phase Transitions

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A short-time dynamic approach to weak first order phase transitions is proposed. Taking the 2-dimensional Potts models as examples, from short-time behaviour of non-equilibrium relaxational processes starting from high temperature and zero temperature states,x pseudo critical points $K^*$ and $K^{**}$ are determined. A clear difference of the values for $K^*$ and $K^{**}$ distinguishes a weak first order transition from a second order one. At the pseudo critical points, pseudo critical exponents can be estimated.

In recent years, much progress has been achieved in non-equilibrium critical dynamics. For example, in a dynamic process in which a system initially at a high temperature or a zero temperature state, is suddenly quenched to the critical temperature or nearby and then evolves dynamically, *short-time* universal scaling behaviour has been found [1, 2]. This phenomenon is rather fundamental. It exists not only in stochastic dynamics described by Langevin equations [1, 3] or Monte Carlo algorithms [2, 4, 5, 6, 7, 8], but also in deterministic dynamics described by fundamental microscopic equations of motion [9]. More interestingly, based on the short-time scaling form, it is possible to determine not only dynamic exponents but also static exponents as well as the *critical* temperature [10, 11]. Since the measurements are carried out in the short-time regime, one does *not* suffer from critical slowing down. Compared with *non-local* cluster algorithms, the short-time dynamic approach does study properties of the original local dynamics and also applies to systems with quenched randomness. For a review, see Ref. [12].

Naturally, it is interesting and attractive to explore possible applications of short-time dynamics to *first* order phase transitions. Especially, due to large correlation lengths and small discontinuities, a *weak* first order transition presents quite similar behaviour as a second order one. It has long been challenging how to distinguish one from the other. Furthermore, *slowing down* in Monte Carlo simulations at first order transitions is even more severe than at second order ones. Non-local cluster algorithms also do not show much more efficiency.

In numerical simulations at first order transitions *in equilibrium*, to locate the transition point one usually searches for the maximums of the specific heat, susceptibility, or a Binder cumulant constructed from energy [13]. For a system with lattice size $L$, these maximums deviate from the real transition point by a power law $1/L^d$. To remove this power law deviation, special techniques have been introduced [14]. With these techniques, first order transition points can be determined rather accurately from moderate lattice sizes, even for weak first order transitions.

To distinguish a first order transition from a second order one, naively one may explore a signal for discontinuity of the order parameter by increasing the lattice sizes. Refined methods are typically based on the *finite size scaling* of the specific heat, susceptibility, order parameter, Binder cumulant of energy, or the transition point, e.g. see Refs. [13, 15, 16, 17, 18, 19, 20, 21]. However, when a first order transition is very weak, it becomes subtle. The lattice sizes one reaches in simulations hardly feel the difference between very large correlation lengths in weak first order transitions and divergent ones in second order transitions. The double peak structure of the energy distribution together with the finite size scaling shows its merit in this respect [22, 23, 24], but further efficient methods are still desired.

In this letter, we propose a short-time dynamic approach to weak first order transitions. The idea is inspired by the existence of two *pseudo* critical points $K^*$ and $K^{**}$ near the weak first order transition point $K_c$ with $K^{**} < K_c < K^*$ [25, 26]. In equilibrium, numerical measurements of $K^*$ and $K^{**}$ are not easy since they are induced by *metastable* states. However, in short-time dynamics $K^*$ and $K^{**}$ can be determined rather accurately from two dynamic processes starting from high temperature and zero temperature states. In second order transitions, $K^*$ and $K^{**}$ overlap with the transition point $K_c$. Therefore, difference of $K^*$ and $K^{**}$ gives a criterion for a weak first order transition.

As examples, we investigate the two-dimensional $q$-state Potts models. The transition point is exactly known at $K_c = \ln(1+\sqrt{q})$. The phase transition is second order for $q \leq 4$ and becomes first order for $q \geq 5$. For small $q$, the first order transitions are weak. Especially, for $q = 5$ the transition is so weak that with standard methods one hardly sees a difference from a second order one.

In second order transitions, it has been shown that at the critical point, short-time behaviour of physical observables is a power law in dynamic processes starting from *both* a random and an ordered state. Away from the critical point, the power law behaviour is modified by a scaling function [12]. We will demonstrate that it is different for first order transitions. An approximate power law behaviour will be observed only at the pseudo critical points $K^*$ and $K^{**}$ in

proper dynamic processes.

We begin our investigation by determining $K^*$ for the 7-state Potts model. For this purpose, we consider a dynamic process in which the system initially in a *random* state, is suddenly quenched to $K_c$ or *above*, then evolves dynamically. We have performed simulations with the heat-bath algorithm. Lattice sizes are $L = 140$ and 280 and maximum updating times are $t_{max} = 2000$ and 6000 respectively. Total samples for averaging are 4600 and errors are simply estimated by dividing the data into four subsamples.

In Fig. 1(a), the second moment $M^{(2)}(t)$ with $L = 280$ is displayed for $K = 1.293562$ ($K_c$), 1.294210 and 1.294857 on a log-log scale. Apparently, at $K_c$ the curve bends *downwards* and does not show a power law behaviour due to the random initial state and the *finite* spatial correlation length in equilibrium. Actually, this already indicates that the transition is first order if we assume $K_c$ is known. What is interesting here is that at a slightly bigger $K$, which we denote by $K^*$, one observes an approximate power law behaviour. The *weaker* the transition is, the *cleaner* the power law behaviour will be. When $K$ becomes bigger than $K^*$, the curve bends *upwards*. Therefore, $K^*$ looks like a critical point [12]. We can not prove that our $K^*$ is the same as the pseudo critical point $K^*$ defined in equilibrium, but we strongly believe so. In equilibrium, $K^*$ is defined as a point at which the system presents approximate scaling behaviour similar to that at a critical point [25, 26].

In our short-time dynamic approach, practically we locate the pseudo critical point $K^*$ by interpolating $M^{(2)}(t)$ among the three simulated $K$'s and searching for the best power law behaviour [11, 12]. In short-time critical dynamics, it has been intensively discussed that universal behaviour emerges only after a time scale $t_{mic}$ which is large enough in microscopic sense. If a Monte Carlo time step (a sweep over all spins on the lattice) is considered to be a microscopic time unit, $t_{mic}$ is typically 10 to some hundred time steps [12]. Similarly, in first order transitions, physical behaviour at *macroscopic* level is presented also only after $t_{mic}$. In the upper part of Fig. 2, $K^*$ obtained with data in a time interval $[t, t_{max}]$ is shown. The results are stable and $K^*$ is clearly above $K_c$. The final value for $K^*$ is estimated to be $K^*_{7s} = 1.293854(29)$. This is consistent with the value $K^* = 1.2945(9)$ given in Ref. [26]. However, the latter can hardly distinguish $K^*$ from $K_c$ within the error.

To determine $K^{**}$, we study a dynamic process in which the system initially in an *ordered* state, is quenched to $K_c$ or *below*, and evolves dynamically. Here we have performed extra simulations for $L = 560$, up to $t_{max} = 6000$. Total samples for $L = 140$, 280 and 560 are 7000, 1500 and 135 respectively. In Fig. 1(b) the magnetisation with $L = 280$ is plotted for $K = 1.2929$, 1.2930 and 1.2931. The curve for $K_c = 1.293562$ (not in the figure) is much above that for 1.2931 and very far from power law behaviour. This is again a signal for a first order transition. The reason is clear. For first order transitions, with an ordered initial state the system will evolve to the ordered phase at $K_c$. However, at the pseudo critical point $K^{**}$ we will observe approximate power law behaviour. Searching for a curve with the best power law behaviour from the three curves in Fig. 1(b), we determine the pseudo critical point $K^{**}$. The results are presented in the lower part of Fig. 2. The values are clearly below $K_c$.

Another interesting observable is the Binder cumulant $U(t) \equiv M^{(2)}(t)/(M(t))^2 - 1$. If a transition is second order, $U(t)$ obeys a power law at the transition point. Therefore it can also be used for the determination of $K^{**}$. Results are included in Fig. 2. Summarising all these measurements leads to $K^{**}_{7s} = 1.293008(7)$.

For the 5-state Potts model, the transition is extremely weak. One should carry out the simulations very carefully. To locate $K^*$, we have first performed simulations with $L = 560$ for $K = 1.174359$ ($K_c$), 1.174946, and 1.175533, up to $t_{max} = 10\,000$ with 1800 samples. The resulting $K^*_{5s} = 1.17445(6)$ is not accurate enough. Therefore another simulation has been carried out at $K = 1.174570$, which is much closer to $K^*$. In Fig. 3(a), the second moments for $K = 1.174359$ ($K_c$) and 1.174570 are displayed. With these data more accurate values for $K^*$ are obtained and collected in the upper part of Fig. 4. We estimate the averaged $K^*_{5s} = 1.174404(7)$.

Similar is the case for the determination of $K^{**}$. We have first performed simulations with an ordered initial state with lattice sizes $L = 280$ and 560 for $K = 1.173890$, 1.174125, and 1.174359 ($K_c$), up to $t_{max} = 10\,000$ with total samples 725. From the data for the magnetisation we estimate a relatively rough $K^{**}_{5s} = 1.17428(9)$. Then we performed simulations at $K = 1.174280$ and 1.174359 ($K_c$) up to $t_{max} = 40\,000$. The results are not sensitive to whether we take $t_{max} = 10\,000$ or 40 000. In Fig. 3(b), the magnetisation at $K = 1.174280$ and 1.174359 ($K_c$) are plotted. From the lower part of Fig. 4, we obtain a final value $K^{**}_{5s} = 1.174322(2)$.

In Table I, all results for $K^*$ and $K^{**}$ have been collected. For both the 7-state and the 5-state Potts model, $K^*$ and $K^{**}$ are clearly above and below the transition point $K_c$ respectively. Our short-time dynamic approach indeed provides a safe criterion for a weak first order transition.

Since our dynamic measurements are carried out in the short-time regime when the spatial correlation length is still short, we can easily control the finite size effect. We also do not have the problem of generating independent configurations and therefore do not suffer from slowing down. After excluding the finite size effect, the measurements are sensitive enough to distinguish a finite but very large spatial correlation length in equilibrium from an infinite one. This is why our method is successful.

With the pseudo critical points in hand, assuming similar scaling laws as in second order transitions [12], one can

estimate corresponding pseudo critical exponents. At $K^*$, e.g,

$$M^{(2)}(t) \propto t^{c_2} \ , \quad c_2 = (d - 2\beta/\nu)/z. \tag{1}$$

At $K^{**}$, for the magnetisation,

$$M(t) \propto t^{-c_1} \ , \quad c_1 = \beta/\nu z, \tag{2}$$

while for the Binder cumulant

$$U(t) \propto t^{c_U} \ , \quad c_U = d/z. \tag{3}$$

Here $d$ is the dimension of the lattice, $\beta$ and $\nu$ are the well known static exponents and $z$ is the dynamic exponent. However, the values of the exponents at $K^*$ and $K^{**}$ can be different. Plotting the observables vs. $t$ in log-log scale, one measures the corresponding exponents from the slopes. The results are given in Table II. Here we should admit that accurate values for complete sets of exponents can not be obtained so easily. One still needs much more careful simulations. An important reason is that $K^*$ and $K^{**}$ are not real critical points. They are also rather close to each other.

In conclusions, we have proposed a short-time dynamic approach to weak first order transitions. From non-equilibrium short-time behaviour of two dynamic processes starting from random and ordered initial states, pseudo critical points $K^*$ and $K^{**}$ are determined. Difference of $K^*$ and $K^{**}$ distinguishes a weak first order transition from a second order one. Since the measurements are carried out in short-time regimes, the method does not suffer from slowing down. Different from many techniques developed in simulations in equilibrium, our method is not based on the finite size scaling.

A simple average of $K^*$ and $K^{**}$ gives a rather good estimate of the transition point $K_c$, especially for very weak transitions. For example, for the 5-state Potts model $(K^* + K^{**})/2 = 1.174363$ and the relative deviation from the exact $K_c$ is only the order of $O(10^{-6})$. It is interesting to investigate how to obtain an accurate $K_c$ for not too weak transitions. Furthermore, how other relevant observables like the specific heat and energy distribution evolve in non-equilibrium dynamics is also an important topic. It is challenging whether from short-time dynamics one can estimate the latent heat and the discontinuity of the order parameter in equilibrium.

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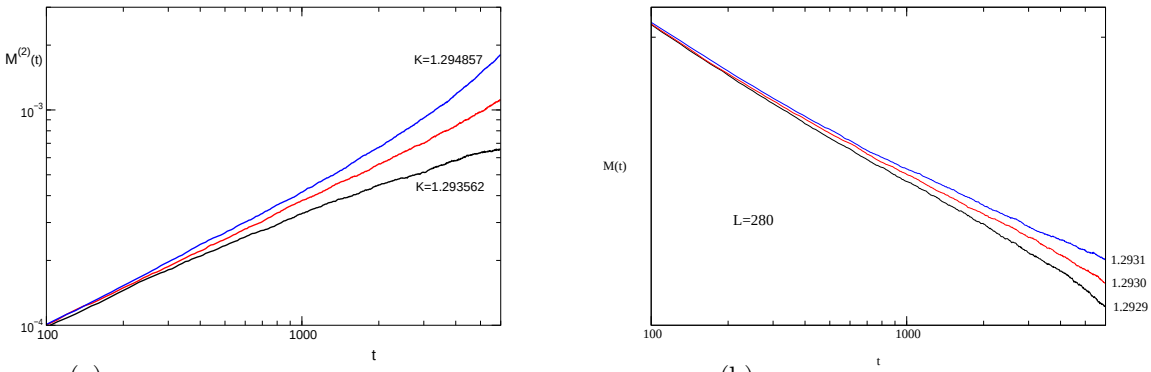


FIG. 1: 7-state Potts model: (a) Second moment $M^{(2)}(t)$ plotted vs. $t$ on log-log scale for $K = 1.293562$ ($K_c$), 1.294210 and 1.294857 (from below) with $L = 280$. (b) Magnetization $M(t)$ plotted vs. $t$ on log-log scale for $K = 1.2929$, 1.2930 and 1.2931 (from below) with $L = 280$.

| | $K^{**}$ | $K_c$ | $K^*$ |
|---|---|---|---|
| $q = 5$ | 1.174322(2) | 1.174359 | 1.174404(7) |
| $q = 7$ | 1.293008(7) | 1.293562 | 1.293854(29) |

TABLE I: Pseudo critical points $K^{**}$ and $K^*$ measured from short-time dynamics for the 5-state and 7-state Potts models, in comparison with the transition point $K_c$.

| | $c_1^{**}$ | $c_U^{**}$ | $c_2^*$ |
|---|---|---|---|
| $q = 5$ | 0.091(2) | 0.93(3) | 0.716(3) |
| $q = 7$ | 0.0239(2) | 0.885(8) | 0.502(5) |

TABLE II: Pseudo critical exponents for the 5-state and 7-state Potts models.

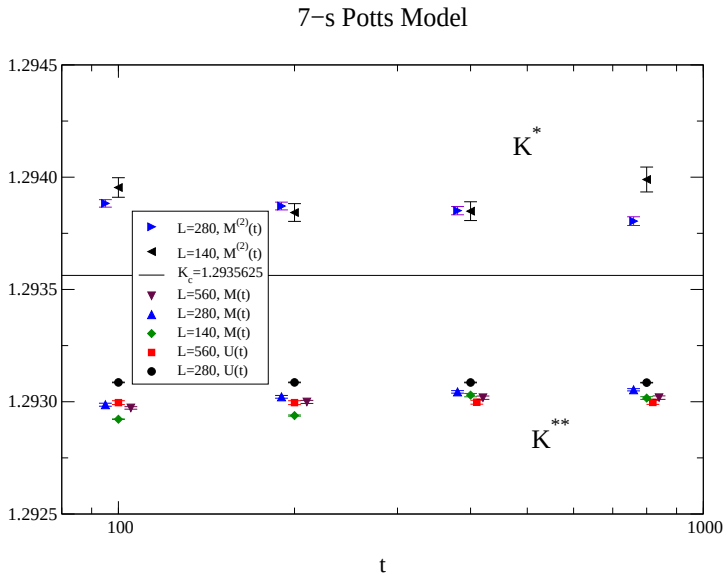


FIG. 2: 7-state Potts model. The upper part shows the values for $K^*$ obtained from $M^{(2)}(t)$ in the interval $[t, t_{max}]$. The lower part shows $K^{**}$ obtained from $M(t)$ and $U(t)$. The line denotes the exact value $K_c$.

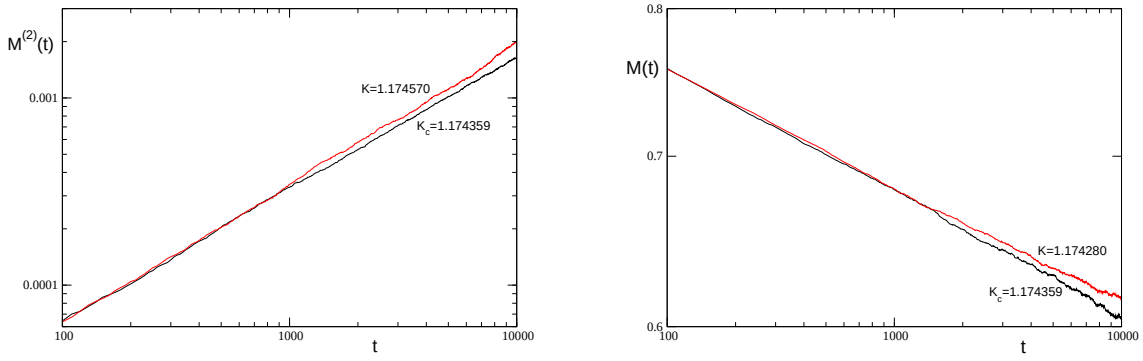


FIG. 3: 5-state Potts model: (a) $M^{(2)}(t)$ plotted vs. $t$ on log-log scale for $K_c = 1.174359$ and $K = 1.174570$ with $L = 560$. (b) $M(t)$ plotted vs. $t$ on log-log scale for $K = 1.174280$ and $K_c = 1.174359$ with $L = 560$.

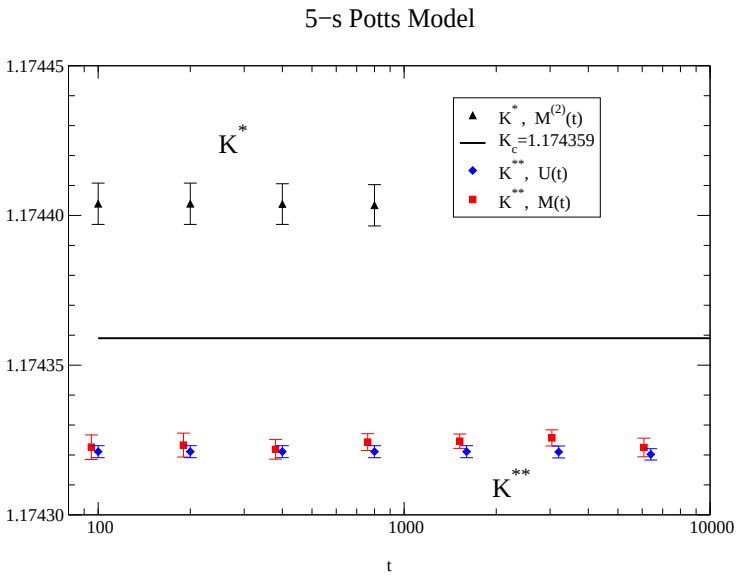


FIG. 4: 5-state Potts model. The upper part shows the values for $K^*$ obtained from $M^{(2)}(t)$ with $L = 560$ in the interval $[t, t_{max} = 10000]$. The lower part shows $K^{**}$ obtained from $M(t)$ with $L = 560$ in the interval $[t, t_{max} = 40000]$. The line denotes the exact value $K_c$.